A Brief Review on Theoretical Models of Deformation Twinning at Locally Distorted Grain Boundaries

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Article history	Abstract
	A brief review of the theoretical models which describe mechanisms of deformation twinning in nanocrystalline and ultrafine-grained materials is presented. In the framework of the models, formation of nanoscale deformation twins occurs at locally distorted grain boundaries that contain fragments being rich with grain boundary dislocations due to preceding severe plastic deformation processes. Within the review, mechanisms of deformation twinning at locally distorted grain boundaries represent (a) the consequent emission of partial dislocation; (b) the cooperative emission of partial dislocations; and (c) the generation of multiplane nanoscale shear.

1. INTRODUCTION

Nanocrystalline (NC) and ultrafine-grained (UFG) materials with unique physical and mechanical properties often demonstrate very high stress and hardness compared to conventional coarse-grained analogues [1]. However, the most NCs show low tensile ductility, which are highly undesirable for their practical applications. It is well known that the conventional lattice dislocation slip is hampered in nanostructured materials due to a large volume fraction occupied by grain boundaries (GBs) which act as effective obstacles for the lattice dislocation slip [1–9]. At the same time, the specific features of the structure of the NC materials provide the action of specific deformation mechanisms [1–9]. According to experimental data, computer simulations and theoretical investigations [7–17] deformation twinning is considered as one of the main deformation mechanism in the nanostructured materials. At the same time, deformation twins are predominantly formed at the GBs in the NC materials, see [12]. For the explanation of this observation, it was suggested that nanoscale

deformation twins form due to the consequent emission of the partial dislocations from the GBs [10–13]. In this case, the partial dislocations should exist on every slip plane at the GB which is hardly possible in the real materials [13]. In order to avoid the discussed discrepancy, Zhu with co-workers [13] suggested a new mechanism of partial dislocation multiplication which realized due to successive processes of dislocation reactions and cross-slips providing existence of the partial dislocations at a GB on every slip plane. However, such reactions are hardly typical in the real materials as specified by very large energy barriers. In order to solve this problem, alternative mechanisms of the deformation twinning that allow the existence of the GB dislocations at the locally distorted GBs on every slip in the NC and the UFG materials was suggested [14–16]. Following the theoretical models [14–16], nanoscale deformation twinning can occur through (a) the consequent emission of the partial dislocation from the locally distorted GBs; (b) the cooperative emission of the partial dislocations from the locally distorted GBs; and (c) the generation of multiplane nanoscale shear at the locally

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distorted GBs. A brief review of these theoretical models will be given in the next sections.

2. MECHANISM OF DEFORMATION TWINNING DUE TO CONSEQUENT EMISSION OF PARTIAL DISLOCATIONS

Consider the first mechanism of deformation twinning through the consequent emission of the partial dislocation from the locally distorted grain boundary (see the theoretical models [14]). Figure 1a illustrates a nanoscale wall configuration *AC* of the GB dislocations formed at GB *AC'* as a result of such GB deformation processes. With this configuration, a nanoscale twin oriented along slip planes {111} is generated and evolves through consequent dislocation emission events as follows.

First, GB dislocations reach the triple junction *A*, and they climb along the GB *AC'* (Figs. 1a,b). These GB dislocations with Burgers vectors b_{gb} form a wall-like configuration *AC* (Figs. 1a,b). The GB dislocations of the wall-like configuration can split into immobile GB dislocations (that stay at the GB *AC'*) and Shockley partial dislocations which are emitted from the GB *AC'* and glide along neighboring glide planes (Figs. 1c–f). This transformation with associated dislocation emission events can be represented as formation of dipoles of partial dislocations characterized by Burgers vectors $\pm b$ and joined by a stacking fault (Figs. 1c–f).

The angle α specifies orientation of {111} slip planes for Shockley dislocations relative to the GB *AC'* plane (Fig. 1c). Within the model [14], Shockley dislocations are edge dislocations of the $(a/6)<11\bar{2}>$ type. They are characterized by the Burgers vector having the modulus of $b = a/\sqrt{6}$. The distance δ between neighboring dipoles of Shockley dislocations is equal to the distance between the neighboring slip planes {111} and is in the following relationship with the crystal lattice parameter a: $\delta = a/\sqrt{3}$. When the *n*th dislocation moves in the grain interior (Figs. 1c–f), a stacking fault of the length p_n is formed behind it (Figs. 1c–f). The stacking fault is characterized by the specific energy (per its unit area) γ which serves as a hampering force for the partial dislocation slip. The dislocation slip is driven by the shear stress τ. The first partial dislocation is emitted from the triple junction *A* (Fig 1c) and moves across the grain interior towards the opposite GB (Fig 1c) when the shear stress reaches its critical value of τ_{c1}. The first partial dislocation moves over some distance p_1 in the grain interior or is stopped by the opposite GB (it depends on the level of the shear stress τ) (Fig. 1c) and creates the stress fields hampering emission of a new dislocation. As a corollary, the critical stress τ_{c2} for emission of the second partial dislocation from the GB *AC'* is larger than that for emission of the first dislocation:
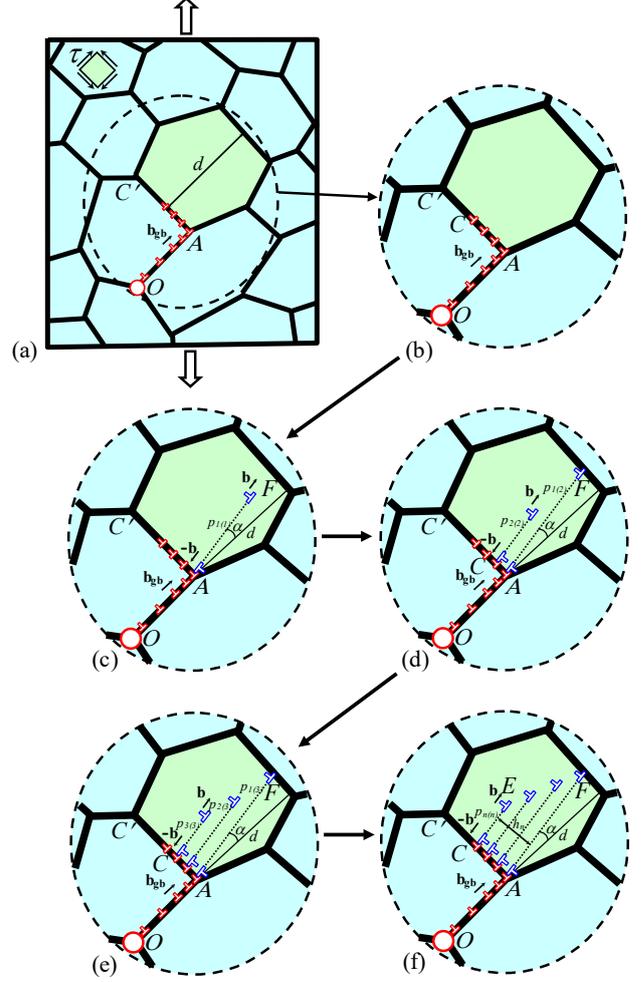
Fig. 1. Model of deformation twinning mechanism through the consequent emission of the partial dislocations from the locally distorted grain boundary. Adapted from Ref. [14].

$\tau_{c2} > \tau_{c1}$. More than that, the second dislocation under the shear stress τ_{c2} does not reach the opposite GB, but moves over some distance p_2 shorter than the distance p_1 moved by the first dislocation (Fig. 1d) as the stress field created by the first dislocation hampers slip of the second partial dislocation. Thus, the critical stress for the emission of the *n*th dislocation is larger than that for the emission of the (*n*–1)th dislocation, and this stress drives slip of the *n*th dislocation over the distance shorter than that moved by the (*n*–1)th dislocation ($p_n < p_{n-1}$).

To analyze the suggested model, we consider the energy characteristics of the nanoscale twin generation due to consequent emission of partial dislocations from locally non-equilibrium GBs (Fig. 1). First, define the conditions which are necessary for the energetically favorable emission of the first partial dislocation which can be represented as formation of a dipole *AF* of partial dislocations with Burgers vectors $\pm b$ (Fig. 1c). Generation of this partial dislocation dipole is characterized by the energy change ΔW_1 (per unit length of the pile-up head dislocation) defined as
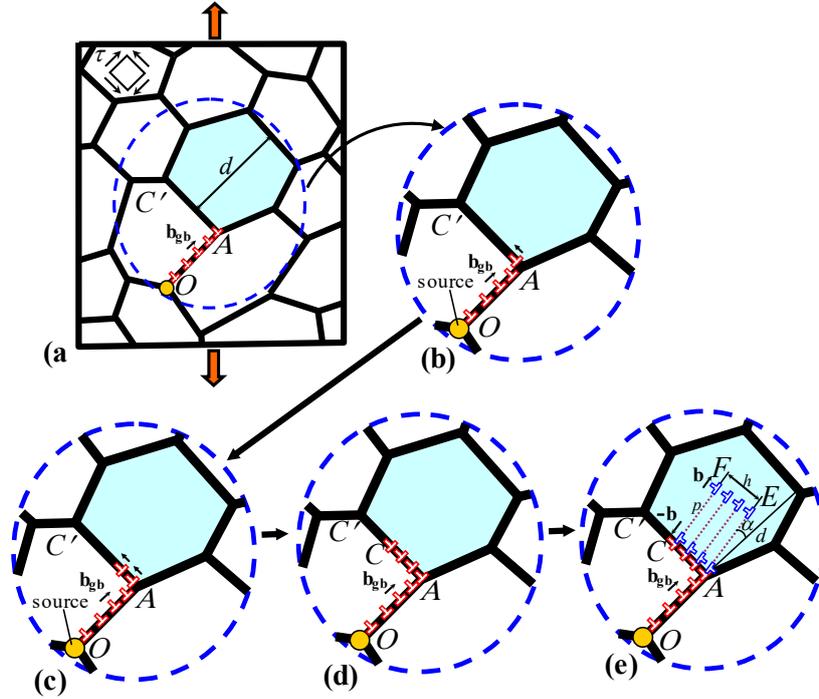
Fig. 2. Model of deformation twinning mechanism through the cooperative emission of the partial dislocations from the locally distorted grain boundary. Adapted from Ref. [15].

$\Delta W_1 = \Delta W_{1,final} - W_{1,initial}$, where $W_{1,final}$ and $W_{1,initial}$ are the energies of the considered defect configuration in its final (Fig. 2c) and initial (Figs. 2a,b) states, respectively. Formation of the dislocation dipole (Fig. 2c) occurs as an energetically favorable process. if $\Delta W_1 < 0$. The energy change in question has five terms [14]:

$$\Delta W_1 = E^b + E^{\Delta-b} + E^{b-b_{gb}} + E_{\tau 1} + E_{\gamma 1}, \tag{1}$$

where E^b is the proper energy of the dipole of the Shockley partial dislocations having Burgers vectors $\pm b$; $E^{\Delta-b}$ is the energy that specifies the interaction between the partial dislocation dipole and the wall AC of GB dislocations; $E^{b-b_{gb}}$ is the energy that specifies the interaction between the partial dislocation dipole and the pile-up OA of GB dislocations; $E_{\tau 1}$ is the work spent by the external shear stress τ on movement of a mobile partial dislocation over the distance p; and $E_{\gamma 1}$ is the energy of the stacking fault formed between the partial dislocations belonging to the dipole AF. Detailed description of all the terms figuring on the right-hand side of Eq. (1) is given in the theoretical paper [14].

Now let us consider the energy characteristics of emission of the nth partial dislocation, for $n > 1$. Emission of the n partial dislocations is equivalent to formation of the nth dislocation dipole (Fig. 1f) in the nanocrystalline solid initially containing the dislocation-pile up and $n-1$ dipoles of partial dislocations and is characterized by the energy change ΔW_n (per unit length of a partial dislocation) defined as $\Delta W_n = W_n - W_{n-1}$, where W_n and W_{n-1} are the energies of the considered defect configuration with n and $n-1$ partial dislocation dipoles, respectively. Formation of the nth dislocation dipole (Fig. 1f) occurs as an energetically favorable process, if $\Delta W_n < 0$. The energy change ΔW_n can be represented as follows [14]:

$$\begin{aligned}\Delta W_n = &\, E_\Sigma^{b(n)} - E_\Sigma^{b(n-1)} + E_\Sigma^{c-b(n)} - E_\Sigma^{c-b(n-1)} + E_\Sigma^{\Delta-b(n)} \\ &- E_\Sigma^{\Delta-b(n-1)} + E_\Sigma^{b-b(n)} - E_\Sigma^{b-b(n-1)} + E_{\gamma\Sigma}^{(n)} - E_{\gamma\Sigma}^{(n-1)} \\ &+ E_{\tau\Sigma}^{(n)} - E_{\tau\Sigma}^{(n-1)}, \end{aligned} \tag{2}$$

where $E_\Sigma^{b(n-1)}$ and $E_\Sigma^{b(n)}$ are the total self-energies of $n-1$ and n partial dislocation dipoles, respectively; $E_\Sigma^{\Delta-b(n-1)}$ is the elastic interaction energy of $n-1$ partial dislocation dipoles with the wall AB of GB dislocations; $E_\Sigma^{\Delta-b(n)}$ is the elastic interaction energy of n partial dislocation dipoles with the wall AB of GB dislocations; $E_\Sigma^{c-b(n-1)}$ and $E_\Sigma^{c-b(n)}$ are the elastic interaction energies of the GB dislocation pile-up OA with $n-1$ and n partial dislocation dipoles, respectively; $E_\Sigma^{b-b(n-1)}$ and $E_\Sigma^{b-b(n)}$ are the sums of the energies specifying the dipole-dipole interaction in situations with $n-1$ and n dislocation dipoles, respectively; $E_{\gamma\Sigma}^{(n-1)}$ and $E_{\gamma\Sigma}^{(n)}$ are the sums of the energies specifying the stacking faults in situations with $n-1$ and n dislocation dipoles, respectively; $E_{\tau\Sigma}^{(n-1)}$ and $E_{\tau\Sigma}^{(n)}$ are the sums of the energies specifying the interaction between the external shear stress τ as well as $n-1$ and n partial dislocation dipoles, respectively.

Detailed description of all the terms figuring on the right-hand side of Eq. (2) is given in the theoretical papers

[14]. The critical stress $\tau_{c(n)}$ is calculated from the equation (2) $\Delta W_n(p_n = 1\,\text{nm}) = 0$.

3. MECHANISM OF DEFORMATION TWINNING DUE TO COOPERATIVE EMISSION OF PARTIAL DISLOCATIONS

The second mechanism of a nanotwin formation is realized through cooperative emission of the partial dislocations from the locally distorted GBs in the NC materials [15]. As in the previous case, the initial defect configuration represents a nanoscale wall of GB dislocations AC located on every (or almost every) slip plane (Figs. 2a–d). The GB dislocations of the wall-like configuration at the GB AC' under the shear stress τ can cooperatively split into immobile GB dislocations (that stay at the GB AC') and Shockley partial dislocations which are cooperatively emitted from the GB AC' and glide along neighboring glide planes (Fig. 2e). The discussed cooperative transformation and associated dislocation emission events can be represented as cooperative formation of dipoles of partial dislocations characterized by Burgers vectors $\pm b$ and joined by stacking faults (Fig. 2e). These stacking faults form a nanoscale twin whose length grows in parallel with slip of the group EF of the partial b-dislocations within the grain interior (Fig. 2e). Such nanotwins have been experimentally observed in nanocrystalline nickel (Ni) [11].

Let us analyze the energy characteristics of the twin formation due to cooperative emission of dislocations from GB in nanomaterials (Fig. 2). The cooperative emission process (Fig. 2) is characterized by the energy difference $\Delta W_n' = W_n' - W'$, where W_n' and W' are the energies of the defect configuration in its final (Fig. 2e) and initial (Fig. 2d) states, respectively (after and before the emission process, respectively). In this situation, the nanotwin generation is energetically favorable, if $\Delta W_n' < 0$. The energy difference $\Delta W_n'$ has the six basic terms [15]:

$$\Delta W_n' = E_{\Sigma n}^{b} + E_{\Sigma n}^{c-b} + E_{\Sigma n}^{\Delta-b} + E_{\Sigma n}^{b-b} + E_{\Sigma n}^{\gamma} + E_{\Sigma n}^{\tau}, \qquad (3)$$

where $E_{\Sigma n}^{b}$ is the total self-energies of n partial dislocation dipoles; $E_{\Sigma n}^{\Delta-b}$ is the elastic interaction energy of n partial dislocation dipoles with the nanoscale wall AC of GB dislocations; $E_{\Sigma n}^{c-b}$ is the elastic interaction energy of the GB dislocation pile-up OA with n partial dislocation dipoles; $E_{\Sigma n}^{b-b}$ is the elastic energy of all the dipole-dipole interactions for n dislocation dipoles; E_n^{γ} is the energy of the twin boundaries; and $E_{\Sigma n}^{\tau}$ is the elastic interaction energy of the external shear stress τ with n partial dislocation dipoles.

Calculation of all the terms figuring on the right-hand side of Eq. (3) is given in the theoretical paper [15]. The critical shear stress $\tau_{c(n)}'$ can be defined as the minimum stress at which the cooperative emission of n partial dislocation from GB is energetically favorable (Fig. 2).

4. MECHANISM OF DEFORMATION TWINNING DUE TO GENERATION OF NANOSCALE MULTIPLANE SHEAR

The third mechanism of nanoscale deformation twin formation is realized through the generation of nanoscale multiplane shear at the locally distorted GBs (Fig. 3) [15,16]. Nanoscale multiplane shear is defined in work [7] as a multiplane ideal shear occurring within a nanoscale region, a three-dimensional region having two or three nanoscopic sizes. Within the model [15,16], a deformation twin is produced under the action of a shear stress τ (Fig. 3) through nanoscale multiplane shear or, in terms of the dislocation theory, through simultaneous nucleation of n dipoles of noncrystallographic dislocations with tiny Burgers vectors $\pm s$ (Figs. 3a–d). The noncrystallographic dislocations of the dipoles are formed at opposite GB fragments, AB and CD, on adjacent {111} planes. The Burgers vectors $\pm s$ of all the dislocations are the same in magnitude and grow simultaneously from zero to the Burgers vectors $\pm b$ of partial dislocations during the nanotwin formation process. In doing so, since there are pre-existent GB dislocations at the GB fragment AB, the noncrystallographic dislocations at the GB fragment AB merge with these pre-existent GB dislocations. As a corollary, during the nanotwin formation process, evolution of the noncrystallographic dislocations at the GB fragment AB manifests itself in evolution of the GB dislocations at this fragment (Figs. 3b–d).

In the case of fcc metals (in particular, copper), the generated dipoles of noncrystallographic partial dislocations formed in adjacent slip planes {111} are assumed to be normal to the grain boundary fragments AB and CD. The region
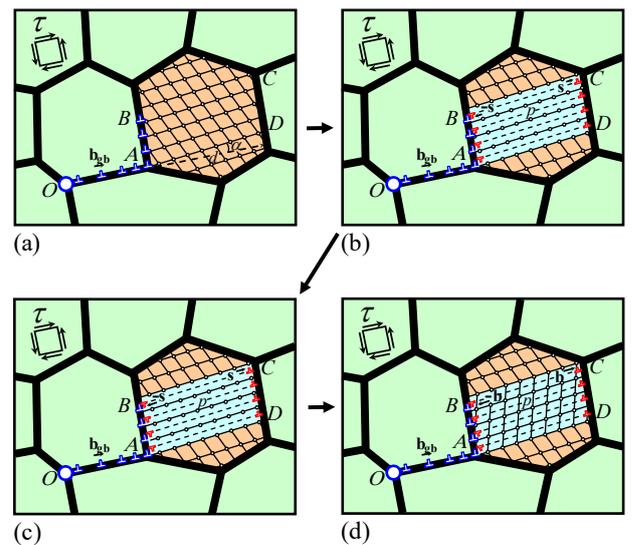
Fig. 3. Model of deformation twinning mechanism through the generation of nanoscale multiplane shear at the locally distorted grain boundary.
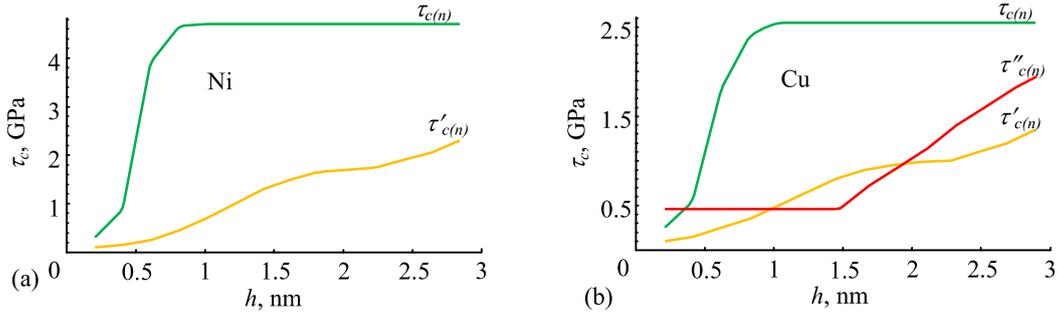
Fig. 4. Comparison of dependences of critical stresses $\tau_{c(n)}$, $\tau'_{c(n)}$ and $\tau''_{c(n)}$ on nanotwin thickness h, for nickel (Ni) (a) and for copper (Cu) (b), respectively.

ABCD (a rectangle with sizes h and p) is subjected to nanoscale multiplane shear which leads to the formation of a nanoscale twin within this region (Fig. 3). In doing so, *AB* length = *CD* length = h and *AD* length = *BC* length = p, where $p = d / \cos\alpha$ and d is the grain size (Fig. 3a).

Let us analyze energetic characteristics of the formation of nanoscale deformation twins through nanoscale multiplane shear initiated at locally distorted GBs in nanocrystalline materials (Fig. 3). In this case, in terms of the dislocation theory, a deformation twin is produced under the action of a shear stress τ through simultaneous nucleation of n dipoles of non-crystallographic dislocations with tiny Burgers vectors $\pm s$ whose magnitudes gradually grow from 0 to b during the nanotwin formation process (Fig. 3).

In general, the energy change ΔW_N that characterizes the nanotwin generation through multiplane nanoscale shear (Fig. 4) has the seven key terms [15]:

$$\Delta W_N = E^s_{\Sigma n} + E^{c-s}_{\Sigma n} + E^{\Delta-s}_{\Sigma n} + E^{s-s}_{\Sigma n} + W_{interior}(s)$$
$$+ W_{AC-BD}(s) + A. \tag{4}$$

Here $E^s_{\Sigma n}$ is the total self-energies of n dipoles of noncrystallographic $\pm s$-dislocations; $E^{c-s}_{\Sigma n}$ is the elastic interaction energy of the pile-up of GB dislocations with n dipoles of noncrystallographic $\pm s$-dislocations; $E^{\Delta-s}_{\Sigma n}$ is the elastic interaction energy of the wall *AB* of GB dislocations with n dipoles of noncrystallographic $\pm s$-dislocations; $E^{s-s}_{\Sigma n}$ is the elastic energy of all dipole-dipole interactions for n dipoles of noncrystallographic $\pm s$-dislocations; $W_{interior}$ denotes the energy of the interior area of the plastically sheared nanocrystal *ABCD*; W_{AD-BC} the energy of the interfaces, *AD* and *BC*, between the sheared region *ABCD* and the neighboring material; A is the work of the external shear stress τ, spent to the plastic shear within the region *ABCD*.

Detailed description of all the terms figuring on the right-hand side of Eq. (4) is given in the theoretical papers [15,16]. The functions $\Delta W_N(s)$ have minimums and maximums in the range of s from 0 to b at low values of τ and monotonously decrease at high values of τ. It is indicated that there are non-zero energy barriers for the formation of deformation twins at low values of τ. Thus, the critical stress $\tau''_{c(n)}$ can be defined as the minimum stress at which the deformation twin formation is a non-barrier process.

5. CRITICAL STRESSES OF DEFORMATION TWIN FORMATION AT GRAIN BOUNDARIES

Let us calculate the critical shear stresses for the various deformation twinning mechanisms at locally distorted GBs in the NC and UFG materials. The dependences of the critical shear stresses $\tau_{c(n)}$ and $\tau'_{c(n)}$, for nickel (Ni), and $\tau_{c(n)}$, $\tau'_{c(n)}$ and $\tau''_{c(n)}$, for copper (Cu) on the nanotwin thickness h are presented in Fig. 4. As it follows from Fig. 4, for Ni, the cooperative emission of partial dislocations from GBs is characterized by the lowest critical shear stress. For Cu the mechanism of the cooperative dislocation emission occurs at the lowest stress level in the case of ultrathin nanotwins generation ($h < 1$ nm). At the same time, for Cu, the mechanism of the nanoscale multiplane shear occurs at the lowest stress level in the range of the nanotwin thickness h from 1 to 2 nm (Fig. 4). For large nanotwins with the thickness $h > 2$ nm, the mechanism of the cooperative emission of partial dislocations from the GBs is the most favorable process in Cu again (Fig. 4).

According to Figure 4, deformation twinning through the cooperative emission of the partial dislocations is the most energetically unfavorable. However, the critical stresses of deformation twinning realization demonstrate very high dependence on the material parameters and the initial state of a locally distorted GB. So, in other situations the consequent emission of the partial dislocations may be favored.

6. CONCLUSIONS

Three theoretical models of nanoscale deformation twinning at the locally distorted GBs in the NC and the UFG materials were described. Within the models, the

deformation twinning mechanisms present (a) the consequent emission of partial dislocations from GBs; (b) the cooperative emission of partial dislocations from GBs; and (c) the generation of multiplane nanoscale shear at GBs. It was shown that the realization of the deformation twinning mechanisms (Figs. 1–3) needs rather high, but realistic levels of the shear stress (Fig. 4). Thus, the suggested mechanisms of the deformation twinning at locally distorted GBs logically explain numerous experimental observations [11,13] of the formation of nanoscale deformation twins at the GBs in the NC and the UFG materials.

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Краткий обзор теоретических моделей деформационного двойникования вблизи локально неравновесных границ зерен

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Аннотация. Представлен краткий обзор теоретических моделей, описывающих механизмы деформационного двойникования в нанокристаллических и ультрамелкозернистых материалах. В рамках моделей образование наноразмерных деформационных двойников происходит на локально неравновесных границах зерен, которые содержат фрагменты, обогащенные зернограничными дислокациями, возникшими в результате предшествующих процессов интенсивной пластической деформации. В рамках обзора механизмы образования двойников на локально неравновесных границах зерен представляют собой (а) последовательную эмиссию частичных дислокаций; (б) кооперативную эмиссию частичных дислокаций; и (в) зарождение множественного наноскопического сдвига.

Ключевые слова: деформация двойникованием; границы зерен; частичные дислокации